Local Conductance and Saturation lengths of Atomic wires dipped in a Conducting medium

Presenter
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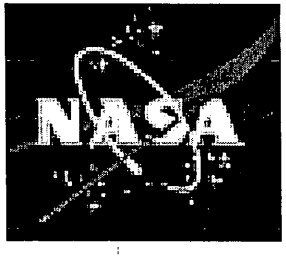

NASA Ames Research Center, Moffet Field, CA, 94035

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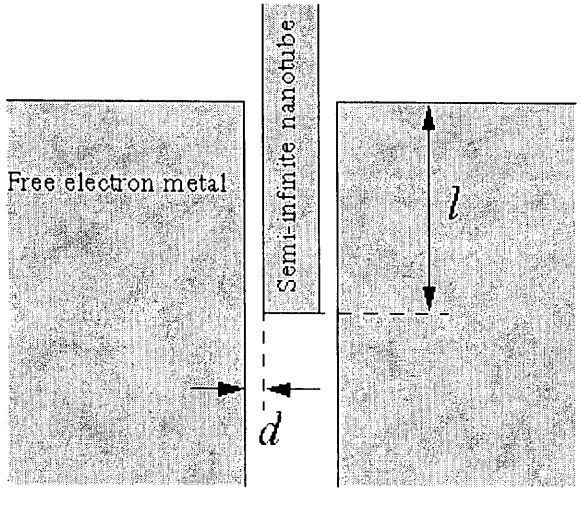
Motivation

- Carbon nanotubes are a promising choice for atomic scale wires.
- Current densities > 10μA/nm^2 have been achieved in nanotubes.
- Crystalline conductor – resistant to electro migration.

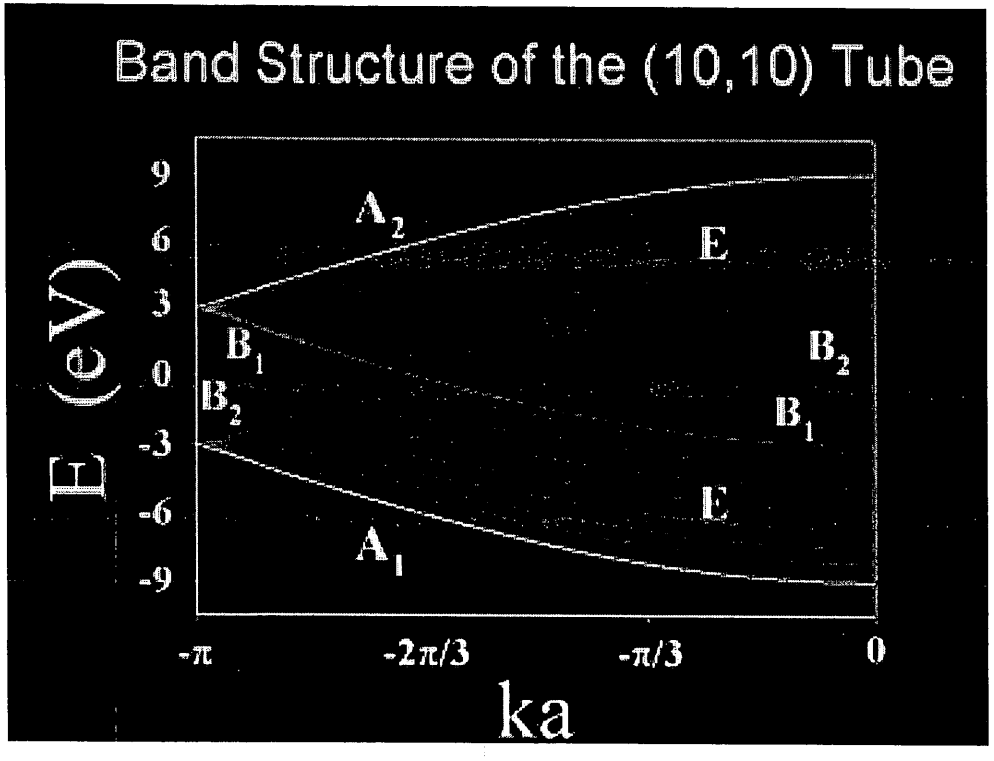
Research topics

- How does the total tube conductance vary with dipping length (l) into the metal electrode?

- How does the current spread locally from the wire to the metal?



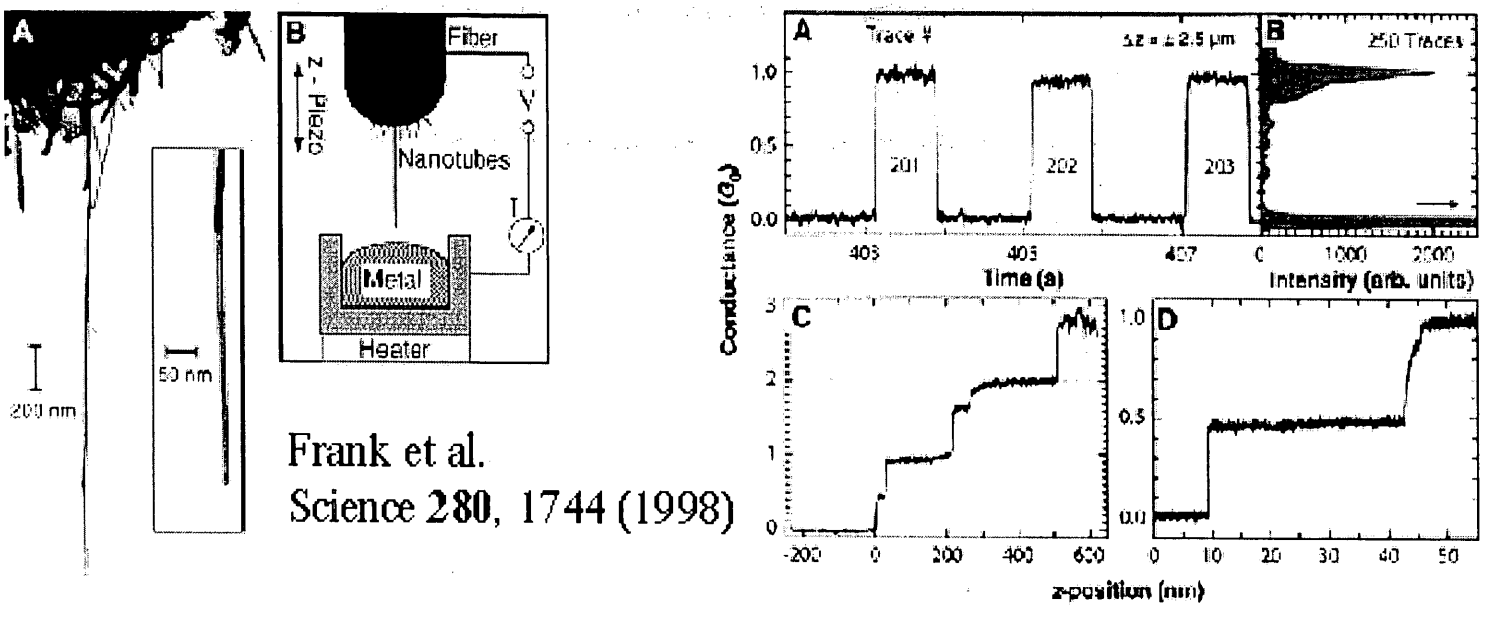
Conducting modes in an armchair nanotube



Smalley Group,
Rice University

- Only two bands (B_1, B_2) cross the Fermi energy.
- These correspond to two conducting modes π and π^*

Experimental Nanotube, Mercury contacts



Frank et al.
Science **280**, 1744 (1998)

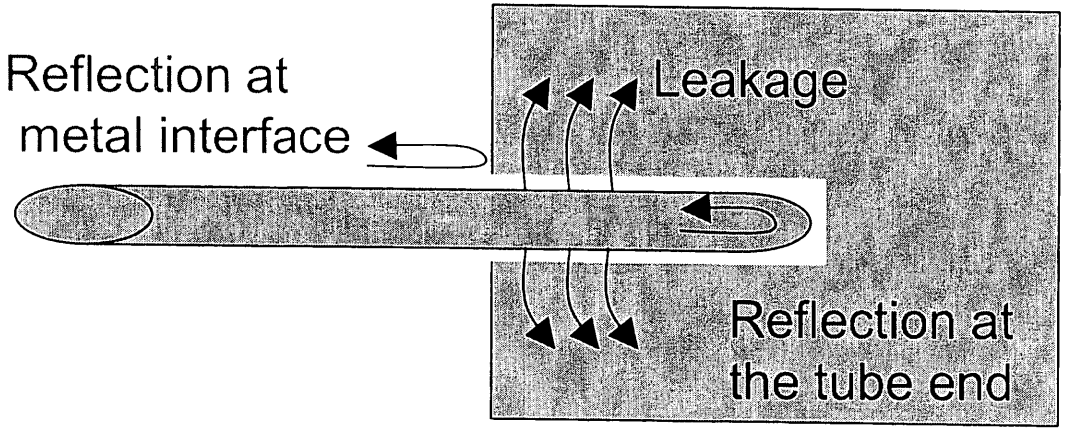
- For moderate dipping lengths ~ 75 nanotube unit cells, conductance saturates to $\sigma = 1G_0$

Metal-Nanotube contact Simulation

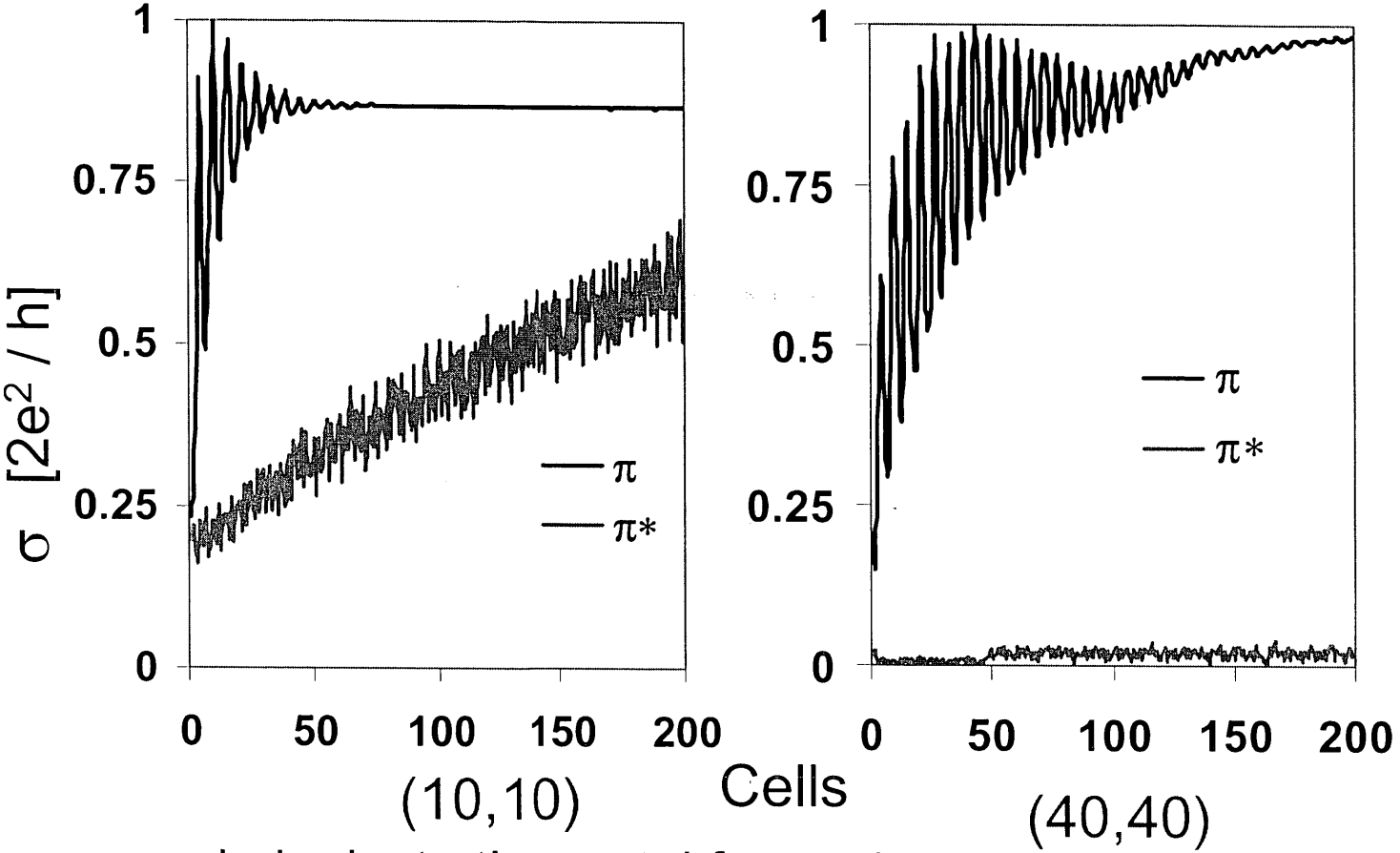
• The metal is modeled as a free electron gas with a fermi energy of 7.1eV corresponding to mercury.

• A nanotube-metal bond distance of 2Å is used. This corresponds to weak coupling.

•A discrete point Hamiltonian is used to model the nanotube
• We calculate the total conductance and local conductance at each nanotube unit cell.

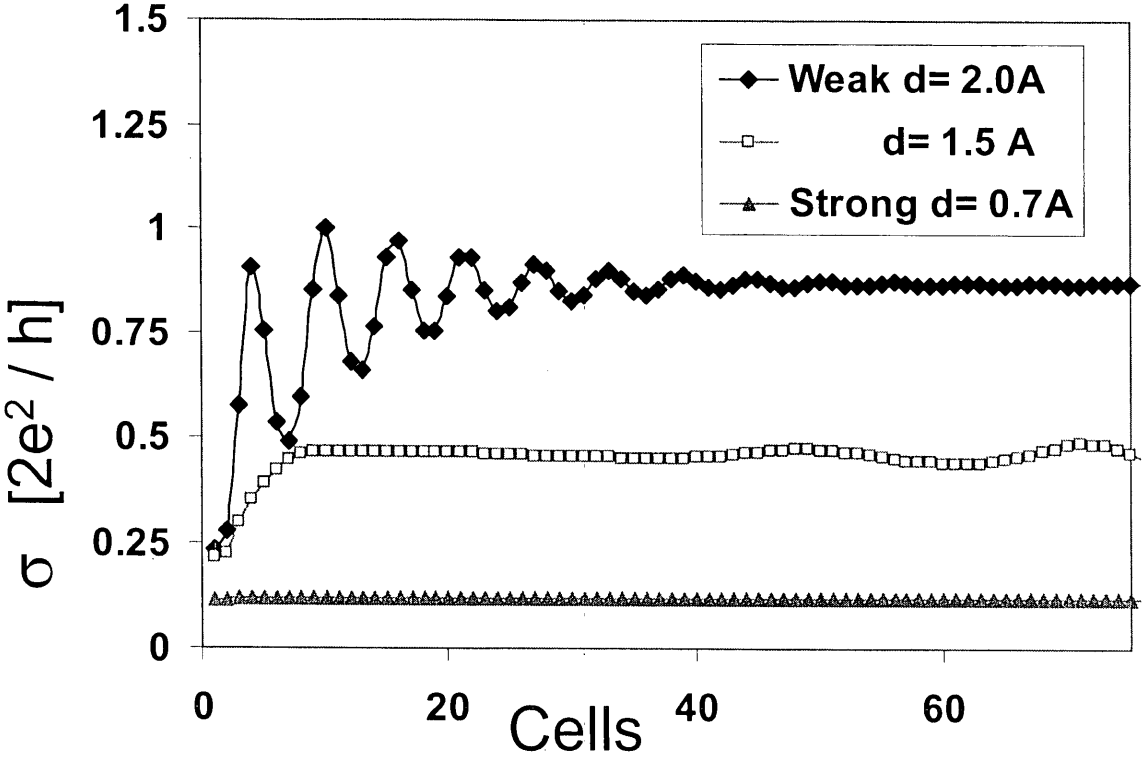


π, π* Mode Conductance



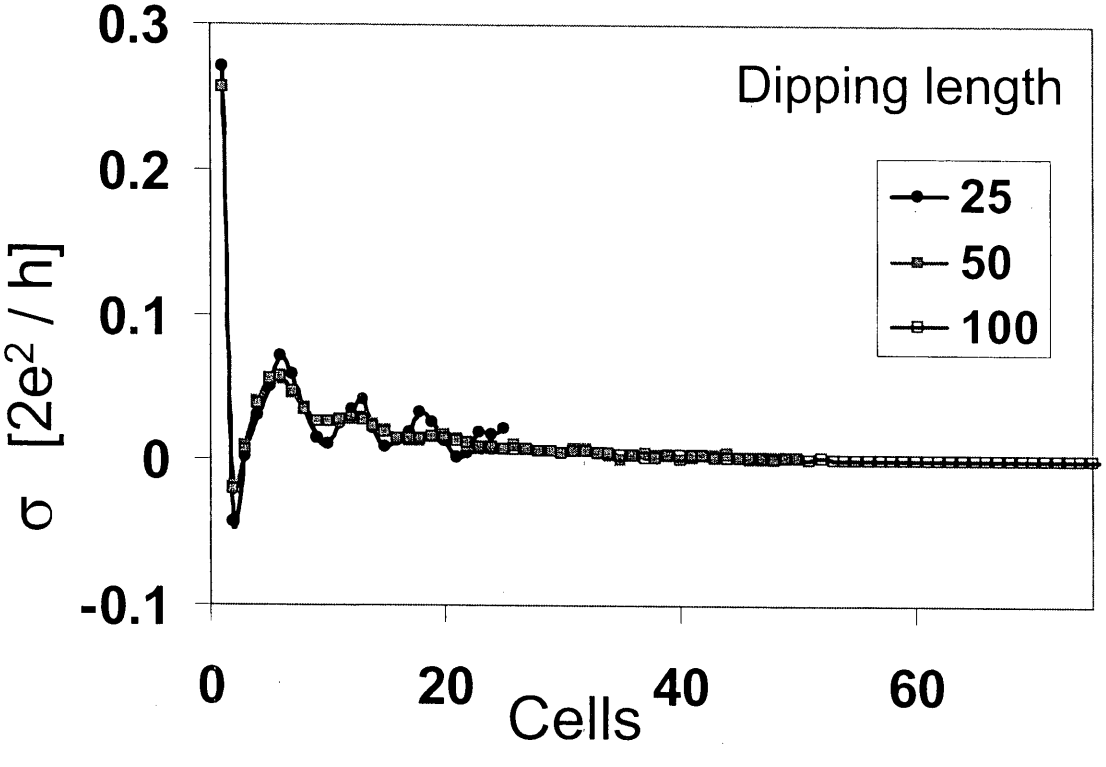
- π mode leaks to the metal faster than π*
- π* mode saturates slower for larger diameter tubes

Total Conductance in a (10,10) tube: π mode



- In the limit of weak coupling to the metal (d > 2 Å) $\sigma \rightarrow 1G_0$
- For strong coupling the conductance saturates immediately to a low value.

Partial Conductance for π mode: (1010) tube



- Oscillations decrease for longer dipping length
- Partial conductance decays very rapidly close to the metal surface

Conclusions

- We conclude that the π is most likely responsible for conduction in experimental mercury-nanotube contacts.

- The total conductance approaches a saturation value as the dipping length is increased.

- There are 2 distinct regimes: Strong and Weak coupling, characterized by saturation conductances of 0 or $1G_o$.

- We have calculated the partial conductance at each nanotube unit cell. The partial conductance exhibits oscillations due to reflection at the end of the tube.